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LLNL-CONF-409083

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December 1, 2008

MRS Fall Meeting
Boston, MA, United States
December 1, 2008 through December 5, 2008

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Structural materials in Gen-IV nuclear reactors will face severe conditions of high operating temperatures, high neutron flux exposure, and corrosive environment. Radiation effects and corrosion and chemical compatibility issues are factors that will limit the materials lifetime. Low-chromium (9-12 Cr wt.%) ferritic martensitic (F/M) steels are being considered as possible candidates because they offer good swelling resistance and good mechanical properties under extreme conditions of radiation dose and irradiation temperature.

The surface chemistry of FeCr alloys, responsible for the corrosion properties, is complex. It exists today a controversy between equilibrium thermodynmic calculations, which suggest Cr depletion at the surface driven by the higher surface energy of Cr, and experimental data which suggest the oxidation process occurs in two stages, first forming a Fe-rich oxide, followed by a duplex oxide layer, and ending with a Cr-rich oxide. Moreover, it has been shown experimentally that corrosion resistance of F/M steels depends significantly on Cr content, increasing with increasing Cr content and with a threshold around 10% Cr, below which, the alloy behaves as pure Fe.

In an attempt to rationalize these two contradicting observations and to understand the physical mechanism behind corrosion resistance in these materials we perform atomistic simulations using our FeCr empirical potential and analyze Cr equilibrium distributions at different compositions and temperatures in single and polycrystalline samples. We analyze the controversy in terms of thermodynamic and kinetic considerations.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.